# MOLECULAR PHYSICS

VOLUME 13

Printed and Published by
TAYLOR & FRANCIS LTD
RED LION COURT, FLEET STREET, LONDON, E.C.4

Copyright 1967 © TAYLOR & FRANCIS LTD

# CONTENTS OF VOLUME 13

## NUMBER 1


Page

Long-range transfer effects in the optical excitations of polyenes. C. Tric and O. Parodi .. .. .. .. .. .. .. .. 1

Dynamic polarization of protons and fluorine nuclei in solutions of free radicals. R. A. Dwek, H. D. W. Hill, J. G. Kenworthy, D. F. S. Natusch and R. E. Richards .. .. .. .. .. .. 27

Relaxation studies. V. A density matrix theory for systems exhibiting second-order hyperfine effects, and the internal motions of phosphorus tetrafluoride. P. W. Atkins .. .. .. .. .. .. 37

Electron spin resonance of an irradiated single crystal of cytosine. J. B. Cook, J. P. Elliott and S. J. Wyard .. .. .. .. .. .. 49

N.M.R. spectra of the $X_nAA'X_n'$ type. Part IV. The use of $^{13}C$ satellites: the spectrum of tetramethyldiphosphine. E. G. Finer and R. K. Harris 65

Electron spin coupling constants for the $a$, $^3A''$ state of formaldehyde. R. N. Dixon .. .. .. .. .. .. .. .. .. 77

Nuclear magnetic resonance spectra of meta-difluorobenzene. S. Mohanty 83

A novel calculation of proton hyperfine coupling constants in the allyl radical. A. Hinchliffe and N. M. Atherton .. .. .. .. .. 89


### Research Note


Paramagnetic resonance in phosphorescent 2-Me naphthalene. H. P. Cleghorn .. .. .. .. .. .. .. .. .. 93


### Errata


Kerr dispersion in alkali metal vapours. L. L. Boyle .. .. .. 97

Theory of hypochromism. R. K. Nesbet .. .. .. .. .. 99


## NUMBER 2


Hyperfine interactions in many atom systems. M. C. Passeggi, A. A. Misetich and T. Buch .. .. .. .. .. .. .. 101

Low energy elastic and resonant exchange cross sections between complex atoms. F. J. Smith .. .. .. .. .. .. .. 121

An expression for the total cross section for molecular scattering in the presence of an angle dependent potential. K. P. Lawley .. .. .. .. 131

Linewidth variations in the electron resonance spectra of transition metal ions undergoing ligand exchange. N. M. Atherton and G. R. Luckhurst 145

Valence states of carbon in $\pi$-electron systems. II. Excited states and ions. H. W. Joy and H. J. Silverstone .. .. .. .. .. .. 149

The electron spin resonance spectrum of $CH_3CO_2^=$ trapped in $\gamma$-irradiated sodium acetate. D. G. Cadena, Jr., V. Mendez and J. R. Rowlands.. 157

Electron spin resonance studies of $VO^{2+}$ in $NH_4Cl$ single crystals. M. Dattatreya Sastry and P. Venkateswarlu .. .. .. .. 161

An SCF calculation of triphenylphosphine. M. Jaro, P. Knowlton, J. E. Bissey, H. Goldwhite and W. R. Carper .. .. .. .. 165

Page

Scalar interactions in phosphorus-31 systems as studied by dynamic nuclear polarization. P. W. Atkins, R. A. Dwek, J. B. Reid and R. E. Richards .. .. .. .. .. .. .. .. .. 175

Electron collision frequencies in polar gases. O. H. Crawford, A. Dalgarno and P. B. Hays .. .. .. .. .. .. .. 181

Research Notes

On a variational principle for the time-dependent Schrödinger equation. R. Prat .. .. .. .. .. .. .. .. .. 193

Zero-field splitting of triplet states of substituted naphthalenes. W. S. Veeman and W. J. van den Hoek .. .. .. .. .. .. 197

Erratum

Off-diagonal constrained variations in open-shell SCF theory. M. Lowe Benston and D. P. Chong .. .. .. .. .. .. .. 199

NUMBER 3

Relaxation studies. VI. Magnetic resonance in the presence of general perturbations. P. W. Atkins and J. N. L. Connor .. .. .. 201

Nuclear magnetic double resonance using very strong decoupling fields. Investigation of an AMX system. T. M. Connor, D. H. Whiffen and K. A. McLauchlan .. .. .. .. .. .. .. .. 221

Electronic spectra of purine and some aminopurines. J. S. Kwiatkowski and J. Wasilewski .. .. .. .. .. .. .. .. 229

The U.V. spectra of dibenz-1,4-dioxin and 1,4-benzdioxin and the E.S.R. spectra of their monopositive ions. A semi-empirical investigation of non-planar $\pi$-electron systems. R. J. Wratten and M. A. Ali .. .. 233

The diphenyl-amino radical dimer. D. A. Wiersma and J. Kommandeur .. .. .. .. .. .. .. .. 241

Molecular motion in liquid bromobenzene and 1,3,5 trideuterobenzene by nuclear magnetic resonance. J. G. Powles and R. Figgins .. .. 253

A re-examination of the I.R. spectrum of dinitrogen trioxide. W. A. Yeranos and M. J. Joncich .. .. .. .. .. .. 263

Nuclear magnetic resonance studies of 1,3-butadienes. Part VI. A theoretical treatment of coupling by pi electrons. A. V. Cunliffe and R. K. Harris .. .. .. .. .. .. .. .. 269

Research Notes

Detection of very small N.M.R. spin coupling constants by resolution enhancement. R. R. Ernst, R. Freeman, Bo Gestblom and T. R. Lusebrink .. .. .. .. .. .. .. .. .. 283

The congruence principle applied to viscosity of *n*-alkane mixtures. B. M. Coursey and E. L. Heric .. .. .. .. .. .. .. 287

Excimer phosphorescence of halogenated benzenes in organic glasses. E. C. Lim and S. K. Chakrabarti .. .. .. .. .. .. 293

Deuteron magnetic resonance in single crystals of copper sulphate penta-deuterate. J. O. Clifford and J. A. S. Smith .. .. .. .. 297

## NUMBER 4

Page

Vibronic interaction in the lower electronic states of benzene. I. Review of the static problem and solution of the pseudo-cylindrical vibronic equations. J. H. VAN DER WAALS, A. M. D. BERGHUIS and M. S. DE GROOT .. .. .. .. .. .. .. .. .. 301

Proton relaxation times in $^{7}$LiCl and $^{6}$LiCl solutions. B. P. FABRICAND and S. S. GOLDBERG .. .. .. .. .. .. .. .. 323

The $^{19}$F magnetic resonance absorption of $CF_4$ and $SF_6$ in their clathrate hydrates. C. A. MCDOWELL and P. RAGHUNATHAN .. .. .. 331

The signs of the vicinal and long-range coupling constants in mercury dimethyl. R. R. DEAN and W. MCFARLANE .. .. .. .. 343

N.M.R. studies of electrolytes in binary solvent mixtures. II. Aqueous mixtures of acetone, acetonitrile, dimethylacetamide, N,N-dimethylformamide, dimethylsulphoxide, dioxane, ethanol, methanol, N-methylformamide, tetrahydrofuran, and tetramethylurea. A. FRATIELLO, R. E. LEE, D. P. MILLER and V. M. NISHIDA .. .. .. .. 349

$^{14}$N chemical shifts in thioamides. P. HAMPSON and A. MATHIAS .. .. 361

Equivalence in anisotropic N.M.R. spectra: the spectrum of ethyl iodide in the nematic phase. C. M. WOODMAN .. .. .. .. .. 365

Molecules and ions in a donor acceptor complex. G. T. POTT and J. KOMMANDEUR .. .. .. .. .. .. .. .. 373

### RESEARCH NOTES

Potential der intramolekularen Wasserstoff-Brückenbindung. K. ARNOLD und G. KLOSE .. .. .. .. .. .. .. .. 391

N.M.R. measurements of large hyperfine splitting constants of radical ions in solution. G. W. CANTERS and E. DE BOER .. .. .. .. 395

The second moment of the broad-line N.M.R. absorption of a proton bonded to a quadrupolar nucleus. G. M. SHELDRICK .. .. .. .. 399

## NUMBER 5

Hyperfine interactions in the gas phase electron resonance spectrum of $^{33}S^{16}O$. A. CARRINGTON, D. H. LEVY and T. A. MILLER .. .. 401

The electron resonance spectrum of a triradical. A. HUDSON and G. R. LUCKHURST .. .. .. .. .. .. .. .. .. 409

The analysis of an ABXY N.M.R. spectrum using sub-spectral and direct methods. P. DIEHL and R. J. CHUCK .. .. .. .. .. 417

Correlation effects in the calculation of ordinary and rotatory intensities. A. E. HANSEN .. .. .. .. .. .. .. .. 425

A precise determination of the H–H and H–F couplings in fluorobenzene. J. E. LOEMKER, J. M. READ, JR. and J. H. GOLDSTEIN .. .. .. 433

The efficient computation of JWKB phase shifts. M. KENNEDY and F. J. SMITH .. .. .. .. .. .. .. .. .. 443

Study of spin density distributions in the radical ions of two non-alternant hydrocarbons by unrestricted Hartree–Fock method: Effect of introducing the variation of $\beta$ and the inclusion of non-neighbour resonance integrals on the spin density values. N. K. RAY and P. T. NARASIMHAN 449

Page

Proton–electron double resonance in organic compounds. R. A. DWEK, O. W. HOWARTH, D. F. S. NATUSCH and R. E. RICHARDS .. .. 457

Molecular two-centre integrals. III. Penetration integrals. A. LOFTHUS 461

All valency electron molecular orbital calculations. I. Dipole moments, spin densities, and $^{19}F$ shielding constants in some fluorobenzenes and fluoronitrobenzenes. D. W. DAVIES .. .. .. .. .. 465

Long-range interactions of alkali metals. A. DALGARNO and W. D. DAVISON .. .. .. .. .. .. .. .. .. 479

RESEARCH NOTES

Long-range interatomic forces. TAI YUP CHANG .. .. .. .. 487

E.S.R. of the charge-transfer triplet state of the durene–tetracyanobenzene complex. HISAHARU HAYASHI, SABURO NAGAKURA and SUEHIRO IWATA 489

Signs of the nuclear spin–spin coupling constants in ammonia. YOSHIFUMI KATO, MINORU MIURA and A. SAIKA .. .. .. .. .. 491

The phase transition of the hard sphere fluid. P. HUTCHINSON .. .. 495

## NUMBER 6

Improved fluid superposition approximation. G. H. A. COLE and A. MORETON .. .. .. .. .. .. .. .. .. 501

A comment on the application of Hartree–Fock perturbation theory to pi-electron systems. A. T. AMOS and J. I. MUSHER .. .. .. 509

Quantenchemische Berechnung der Energiehyperfläche von $H_2+HeH^+$, I. I. FUNKE, H. PREUSS und G. DIERCKSEN .. .. .. .. .. 517

Spectral analysis of the $^1H$, $^{19}F$ and $^{13}C$ N.M.R. spectra of fluorobenzene. T. F. PAGE, JR. .. .. .. .. .. .. .. .. 523

Kerr dispersion of atomic sodium and lithium. M. P. BOGAARD, A. D. BUCKINGHAM and B. J. ORR .. .. .. .. .. .. .. 533

The substituent effect on ring proton coupling constants in 3-substituted pyridines. D. G. DE KOWALEWSKI and E. C. FERRÁ .. .. .. 547

Approximate *ab initio* calculations on polyatomic molecules. D. B. COOK, P. C. HOLLIS and R. MCWEENY .. .. .. .. .. .. 553

The E.P.R. spectrum of an unsaturated ketone negative ion. HSI-LIN JIN CHEN and M. BERSOHN .. .. .. .. .. .. .. 573

Integral coalescence conditions. D. P. CHONG .. .. .. .. 577

RESEARCH NOTES

Electron resonance of phosphorescent benzene in a single crystal. M. S. DE GROOT, I. A. M. HESSELMANN and J. H. VAN DER WAALS .. .. 583

$^{13}C$ spin–spin coupling to group IV elements in symmetrical molecules. W. MCFARLANE .. .. .. .. .. .. .. .. 587

Notes on the E.S.R. spectrum of hydrogenated pyridine. T. YONEZAWA, H. NAKATSUJI, T. KAWAMURA and H. KATO .. .. .. .. 589

Index of authors (with the titles of papers) .. .. .. .. .. 591